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STUDIES IN QUALITY IMPROVEMENT I:
DISPERSION EFFECTS FROM FRACTIONAL
DESIGNS

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ABSTRACT

Fractional factorial designs have been used successfully in industry and elsewhere to detect and estimate sparse factor effects. The effects usually envisioned measure changes in location associated with the experimental factors. In this paper we consider the possibility of detecting and estimating sparse dispersion effects measuring changes in variance associated with the factors.

AMS(MOS) Subject Classifications: 62K15

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SIGNIFICANCE AND EXPLANATION

Unreplicated fractional factorial designs are frequently employed as screening designs in industrial experimentation. Current methods of analysis are primarily concerned with determining the effect of experimental variables on the mean value or location of the response y in terms of the usual main effects and interactions which we will here call location effects. We consider in this paper the possibility that the variables may also affect the variance of y analogously through dispersion effects. The nature of the alias relationships between location and dispersion effects is discussed and a method developed for identification of dispersion effects when location effects are also present.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

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DISPERSION EFFECTS FROM FRACTIONAL DESIGNS

George E.P. Box and R. Daniel Meyer*

1. INTRODUCTION

Table 1 shows in summary a highly fractionated two-level factorial design employed as a screening design in an off-line welding experiment performed by the National Railway Corporation of Japan (Taguchi and Wu, 1980). To the right of the table is shown the observed tensile strength of the weld, one of several quality characteristics measured.

The authors assumed that, in addition to main effects only the interactions AC, AG, AH, and GH might be present. On that supposition, all nine main effects and the four selected two-factor interactions can be separately estimated by appropriate orthogonal contrasts and the two remaining contrasts corresponding to the columns labelled e_1 and e_2 measure only experimental error. In the last row of the table are shown the grand average and the fifteen effect contrasts calculated in the usual manner. In this paper these will be referred to as "location" effects. They are plotted in a dot diagram below the table. A normal probability plot (Daniel 1959, 1976) shows thirteen effects roughly following a straight line with main effects B and C, falling markedly off the line. This suggests that, over the ranges studied, only factors B and C affect tensile location by amounts not readily attributed to noise.

On the assumption, then, that B and C are the only important location effects, the sixteen runs could be regarded as four replications of a 2^2 factorial design in factors B and C only. However when the results are plotted in Figure 1 so as to reflect this, inspection suggests the existence of a dramatic effect of a different kind apparently not

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A: Kind of Welding Rods
 B: Period of Drying
 C: Welding Material
 D: Thickness
 E: Angle
 F: Opening
 G: Current
 H: Welding Method
 J: Preheating

Factor	I	D	H	G	F	GH	AC	A	E	AH	θ_2	AG	J	B	-C	Tenile strength kg/mm
Column Number	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	+	+	-	+	-	+	+	-	+	+	+	+	+	-	+	43.7
2	+	+	-	-	-	+	+	+	-	+	+	+	+	-	-	40.2
3	+	+	+	-	-	+	-	-	+	-	-	+	+	+	-	42.4
4	+	+	+	+	-	-	-	-	-	-	-	+	+	+	+	44.7
5	+	+	-	+	+	+	-	-	+	+	+	-	+	+	-	42.4
6	+	+	-	-	+	+	-	-	-	+	+	-	-	+	+	45.9
7	+	+	+	+	+	+	+	-	+	-	-	+	+	-	+	42.2
8	+	+	+	+	+	+	+	-	-	-	-	-	-	+	-	40.6
9	+	+	-	-	-	+	+	+	+	-	-	-	+	+	+	45.5
10	+	+	-	-	-	+	+	+	+	-	-	-	+	+	+	43.6
11	+	+	+	+	-	+	-	+	+	+	+	-	-	-	-	40.6
12	+	+	+	+	-	-	-	+	+	-	-	-	+	-	+	44.0
13	+	+	-	+	+	+	-	+	+	-	-	+	+	+	-	40.2
14	+	+	-	+	+	+	-	+	+	-	-	+	+	+	-	42.5
15	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	46.5
Effect	43.0	.13	-.15	-.30	-.15	.40	-.03	.38	.40	-.05	.43	.13	.13	-.30	2.15	3.10

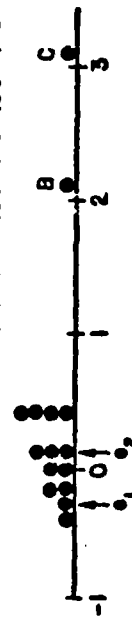


Table 1. A fractional two-level design used in a welding experiment with the estimated location effects plotted as a dot diagram. For convenience in later discussion the design layout has been recast so that the columns as well as the rows follow standard factorial order. Also the preheating variable has been labelled J so that, as is customary, the letter I may be used for the initial column of plus signs.

previously noticed. When factor C is at its minus level, corresponding to the use of an alternative material, the spread of the data appears much larger than when C is at its plus level. Thus in addition to detecting shifts in location due to B and C, the experiment may also have detected what we will call a dispersion effect due to C.

This, of course, is not the only possible explanation of the data. If, instead of adopting the assumptions of the authors, it has been supposed, for example, that all two-factor interactions might be appreciable, then, because of the identity $-BCD = 1 \times 14 \times 15 = I$ in the defining relation of the design, the large contrasts associated with columns 14 and 15 could have been due to B and C as postulated or alternatively to B and BD or to C and CD. The data might also be accounted for by supposing that certain of the tested factors other than B and C affected C only at its minus level. Analysis of the eight runs made at the minus level of C do not support any simple explanation of this kind. However screening designs should normally be employed in a sequential process of investigation where the alternative possibilities which they offer may be resolved in subsequent experimentation. (See, for example, the discussion of Tippett's cotton experiment on pages 88-90 of Fisher (1966) also Box, Hunter and Hunter 1978.) In an ongoing investigation therefore such possibilities ought to be considered for further study. We shall pursue the implications of the simplest explanation here while inviting the reader to bear all the above provisos in mind.

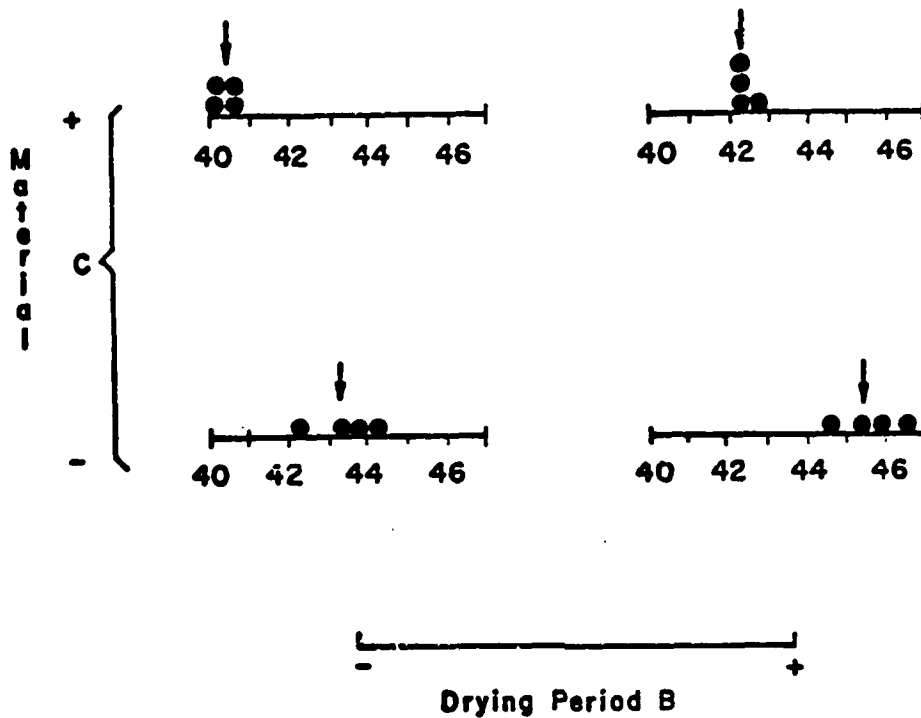


Figure 1. Welding experiment data presented as four replicates of a 2^2 factorial design in factors B and C only. Arrows indicate sample averages.

2. DISPERSION EFFECTS

Fractional arrangement and other orthogonal arrays introduced by Finney (1975), Plackett and Burman (1946) and Rao (1947) have frequently been used in industry: see for example Davies (1954), Daniel (1976), Box, Hunter & Hunter (1978). In particular they are employed as screening designs when it is believed that the large effects it is desired to detect come from only a small number of the tested factors. This may be called the hypothesis of effect sparsity. The tensile data suggests the general possibility that the use of unreplicated fractional designs might provide an economical way of detecting sparse dispersion effects as well as sparse location effects. This idea is pursued in the remainder of this paper. The procedures we discuss are for the identification stage of the problem-solving iteration (see for example Box & Jenkins, 1976) suggesting tentatively which factors might have location and which dispersion effects. Efficient maximum likelihood estimation for fitting an identified model is briefly discussed at the end of the paper.

Consider again the design of Table 1. There are 16 runs from which 16 quantities--the average and 15 effect contrasts--have been calculated. Now if we were interested in possible dispersion effects we could also calculate 15 variance ratios. For example, for the i 'th column we could compute the sample variance $s^2(i-)$ from the eight observations associated with a minus sign and compare it with the sample variance $s^2(i+)$ from the eight observations associated with a plus sign, to provide the ratio $F_i = s^2(i+)/s^2(i-)$. If this is done for the fifteen contrast columns of welding data the values for $\ln F_i$ given in Figure 2(a) are obtained.

It will be recalled that in the earlier analysis a large dispersion effect was associated with factor C (column 15). However in Figure 2(a) the dispersion effect for this factor is not especially extreme, instead the effect for factor D (column 1) stands out from all the rest. We will see how this may be accounted for by the aliasing of location and dispersion effects which we now consider in a preliminary way.

Since the sixteen location effects are obtained by non-singular linear transformation of the original sixteen data values, calculated dispersion effects must be functions of the location effects. The general nature of the location-dispersion aliasing is explained in the section 3 which follows. It is shown that each dispersion effect is a ratio of *sums of* sums and differences of the location effects. For immediate illustration equation (1) shows the identity that exists for the F ratio associated with factor D, and hence for column 1, of the design. In this expression \hat{i} is used to indicate the location contrast associated with the i th column.

$$F_D = F_1 = \frac{(\hat{2}+\hat{3})^2 + (\hat{4}+\hat{5})^2 + (\hat{6}+\hat{7})^2 + (\hat{8}+\hat{9})^2 + (\hat{10}+\hat{11})^2 + (\hat{12}+\hat{13})^2 + (\hat{14}+\hat{15})^2}{(\hat{2}-\hat{3})^2 + (\hat{4}-\hat{5})^2 + (\hat{6}-\hat{7})^2 + (\hat{8}-\hat{9})^2 + (\hat{10}-\hat{11})^2 + (\hat{12}-\hat{13})^2 + (\hat{14}-\hat{15})^2} \quad (1)$$

This equation shows in particular how the extreme value for F_D , can be accounted by the location effects $\hat{B} = \hat{14} = 2.15$ and $-\hat{C} = \hat{15} = 0.10$ whose squared sum and squared difference appear respectively in its numerator and denominator.

A natural way to try to eliminate such aliasing is to compute variances from the residuals obtained after least squares modelling of large location effects. We show in Section 3 that after such elimination alias relations such as equation 1 remain of the same form but with location effects from eliminated variables removed. Dispersion effects \hat{F}_1 calculated from residuals after eliminating the location effects of B and C are shown in Figure 2(b). It is seen that an extreme dispersion effect is now associated with C agreeing with our earlier analysis.

Column	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Effect	D	H	-e ₁	G	-F	GH	-AC	A	-E	AH	e ₂	AG	J	B	-C
$\ln F_i$	2.72	-.14	-.10	.41	.37	.50	.26	.25	.23	.37	.42	.17	.13	.13	.51

$\ln \hat{F}_i$	-.03	1.81	.23	1.06	-.89	.64	-.70	-.71	.65	-.90	1.07	.12	1.63	-.19	2.92
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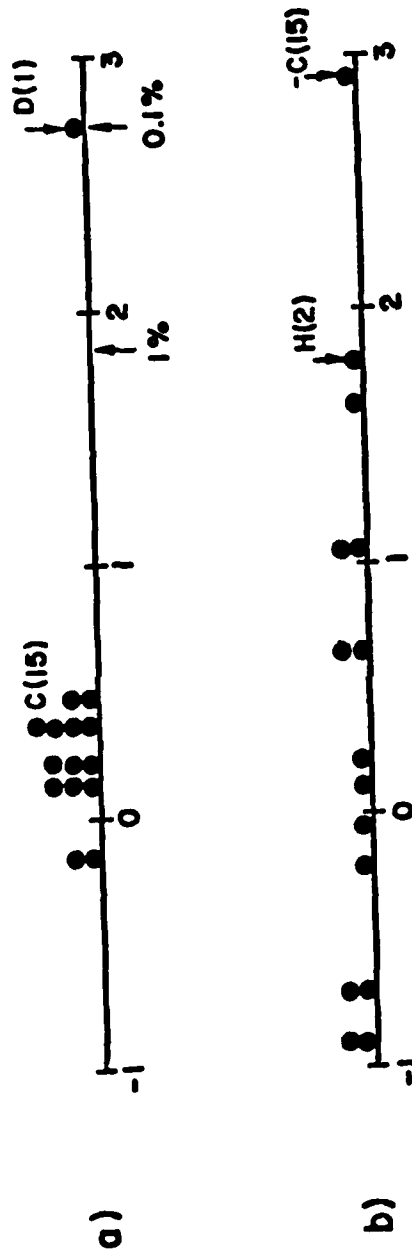


Figure 2. Welding experiment: log dispersion effects (a) crude dispersion effects $\ln F_i$ before elimination of location effects B and C, (b) corrected dispersion effects $\ln \hat{F}_i$ after elimination of location effects B and C. Normal theory significance levels are shown to provide a rough indication of size; note, however, needed assumptions for the usual F test are not satisfied.

3. DISPERSION AND LOCATION ALIASING

3.1. Identities Existing Between Dispersion and Location Effects

In order to study the identity relations existing between location and dispersion effects consider an $n \times n$ orthogonal array with $n = 2^q$ columns of -1 's and $+1$'s labelled x_0, x_1, \dots, x_{n-1} . Let $x_0 = 1$ be a column of $+1$'s and the remaining columns delineate the usual contrasts for the main effects and interactions of a 2^q factorial design. In general we suppose that the array is to be used either as a 2^{k-p} fractional or as a full factorial to test k factors, so that $q = k - p$ with $p \geq 0$.

To generate the columns of a 2^q orthogonal array it is convenient to begin by writing a full factorial for q letters employing Yates' standard order columnwise. We then label columns from zero to $n-1$ (as illustrated below and in Table 1 for $q = 3$ and $q = 4$ respectively). In practice a design with $n = 8$ would usually be too small to allow variance effects to be usefully studied. We employ it here only to illustrate the argument.

0	1	2	3	4	5	6	7
I	A	B	AB	C	AC	BC	ABC
+1	-1	-1	+1	-1	+1	+1	-1
+1	+1	-1	-1	-1	-1	+1	+1
+1	-1	+1	-1	-1	+1	-1	+1
+1	+1	+1	+1	-1	-1	-1	-1
+1	-1	-1	+1	+1	-1	-1	+1
+1	+1	-1	-1	+1	+1	-1	-1
+1	-1	+1	-1	+1	-1	+1	-1
+1	+1	+1	+1	+1	+1	+1	+1

As is well known an array generated in this way may be used as a full factorial or as a fractional design. For example, associating three factors with columns 1, 2, 4 above reproduces the 2^3 factorial, four factors associated with columns 1, 2, 4, 7 produces a 2^{4-1}_{IV} fractional, seven factors associated with columns 1 through 7 produces a 2^{7-4}_{III} fractional. The roman subscript is used to denote the design resolution: that is the length of the shortest word in the defining notation (see, for example Box & Hunter (1961)).

Now because the columns x_0, x_1, \dots, x_{n-1} form a group closed under multiplication defined such that the product column x_{ij} has for its u th element $x_{iju} = x_{iu}x_{ju}$, any such product column must be a column of the original array.

Consider now the elements of a column $\frac{1}{2}(x_0 \pm x_i) (i \neq 0)$; these are

$$\frac{1}{2}(x_{0u} - x_{iu}) = \begin{cases} +1 & \text{if } x_{iu} = -1 \\ 0 & \text{if } x_{iu} = +1 \end{cases} \quad (2)$$

$$\frac{1}{2}(x_{0u} + x_{iu}) = \begin{cases} 0 & \text{if } x_{iu} = -1 \\ +1 & \text{if } x_{iu} = +1 \end{cases}$$

Also the elements of a column $\frac{1}{2}(x_j \pm x_{ij})$ are

$$\frac{1}{2}(x_{ju} - x_{iju}) = \frac{1}{2}x_{ju}(x_{0u} - x_{iu}) = \begin{cases} x_{ju} & \text{if } x_{iu} = -1 \\ 0 & \text{if } x_{iu} = +1 \end{cases} \quad (3)$$

$$\frac{1}{2}(x_{ju} + x_{iju}) = \frac{1}{2}x_{ju}(x_{0u} + x_{iu}) = \begin{cases} 0 & \text{if } x_{iu} = -1 \\ x_{ju} & \text{if } x_{iu} = +1 \end{cases}$$

To see how this may be used to study location and dispersion aliasing consider for illustration the 2^3 design. Suppose we wished to compare variances at the lower and upper level of factor $C = x_4$. Then the columns $\frac{1}{2}(x_j - x_{4 \cdot j})$ are

	$j = 0$	4	1	5	2	6	3	7
	+1	-1	-1	+1	-1	+1	+1	-1
	+1	-1	+1	-1	-1	+1	-1	+1
	+1	-1	-1	+1	+1	-1	-1	+1
	+1	-1	+1	-1	+1	-1	+1	-1
$\frac{1}{2}(x_j - x_{4 \cdot j})$	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0

In general for every i the columns $(x_j - x_{i \cdot j})$ will appear in $\frac{n}{2} = 2^{q-1}$ pairs identical apart from sign. Now suppose data $y = (y_1, \dots, y_u, \dots, y_n)$ are available and

let $\hat{j} = \chi'x_j$ from which the estimated effect of factor j may be obtained by dividing by an appropriate constant. Then for every i the quantities $\chi'(x_j - x_{i \cdot j}) = \hat{j} - i \cdot \hat{j}$ provide an exhaustive set of $n/2$ linearly independent contrasts of those $n/2$ observations y_u for which $x_{iu} = -1$. Correspondingly, the columns $x_j + x_{i \cdot j}$ provide a similar set of contrasts for the remaining observations for which $x_{iu} = +1$. Denote by $S(i-)$ and $S(i+)$ the sums of squares of the y_u for which $x_{iu} = -1$ and $+1$ respectively. Then

$$S(i-) = \frac{1}{n} \sum_{j=0}^{n-1} [1/2 \chi'(x_j - x_{i \cdot j})]^2 = \frac{1}{n} \sum_{j=0}^{n-1} \left(\frac{\hat{j} - i \cdot \hat{j}}{2} \right)^2 \quad (4)$$

$$S(i+) = \frac{1}{n} \sum_{j=0}^{n-1} [1/2 \chi'(x_j + x_{i \cdot j})]^2 = \frac{1}{n} \sum_{j=0}^{n-1} \left(\frac{\hat{j} + i \cdot \hat{j}}{2} \right)^2 .$$

For example, returning for illustration to the 8×8 array discussed above

$$\begin{aligned} S(4-) &= y_1^2 + y_2^2 + y_3^2 + y_4^2 \\ &= \frac{1}{8} \left[\left(\frac{\hat{0}-\hat{4}}{2} \right)^2 + \left(\frac{\hat{1}-\hat{5}}{2} \right)^2 + \left(\frac{\hat{2}-\hat{6}}{2} \right)^2 + \left(\frac{\hat{3}-\hat{7}}{2} \right)^2 + \left(\frac{\hat{4}-\hat{0}}{2} \right)^2 + \left(\frac{\hat{5}-\hat{1}}{2} \right)^2 + \left(\frac{\hat{6}-\hat{2}}{2} \right)^2 + \left(\frac{\hat{7}-\hat{3}}{2} \right)^2 \right] \\ &= \frac{1}{4} \left[\left(\frac{\hat{0}-\hat{4}}{2} \right)^2 + \left(\frac{\hat{1}-\hat{5}}{2} \right)^2 + \left(\frac{\hat{2}-\hat{6}}{2} \right)^2 + \left(\frac{\hat{3}-\hat{7}}{2} \right)^2 \right] \\ &= \frac{1}{4} \left[\left(\frac{\hat{I}-\hat{C}}{2} \right)^2 + \left(\frac{\hat{A}-\hat{AC}}{2} \right)^2 + \left(\frac{\hat{B}-\hat{BC}}{2} \right)^2 + \left(\frac{\hat{AB}-\hat{ABC}}{2} \right)^2 \right] . \end{aligned} \quad (5)$$

3.2. Elimination of Location Effects

The sums of squares in (4), (5) would be appropriate to compute dispersion effects only if it could be assumed that all the location effects, including the overall mean, were known to be zero. If this were not the case then the sums of squares $S(i-)$ and $S(i+)$ could be inflated by location effects. To remove such effects we can replace the y_u 's in (5) by residuals $y_u - \hat{y}_u$ obtained after eliminating all suspected location effects, including the mean, by least squares. Since for this mode of estimation the

vector of residuals is orthogonal to each column vector corresponding to an eliminated variable, it follows that the identity relation for a sum of squares calculated from such residuals is still expressed by equation (4) but with all estimated contrasts corresponding to eliminated variables set equal to zero.

3.3. Expected Values of Sums of Squares of Residuals

Further understanding is gained by considering the expected values of $S(i-)$ and $S(i+)$ under various circumstances. Suppose a difference in variance might exist associated with the level of the single column x_1 and the sums of squares $S(i-)$ and $S(i+)$ are computed from (4) but with y_u replaced by residuals after a number of location effects have been eliminated. Then, after setting to zero all the elements \hat{j} and $i \cdot \hat{j}$ in (5) which correspond to eliminated variables, suppose there are l cases where bracketed pairs $(\hat{j}, i \cdot \hat{j})$ have been eliminated and m cases where only one element of a bracketed pair has been eliminated so that there remains $\frac{n}{2} - l - m$ complete bracketed pairs.

For a bracketed pair

$$E\left[\frac{2}{n} \left\{ \frac{1}{2} (\hat{j} - i \cdot \hat{j}) \right\}^2\right] = \sigma^2(i-) \quad (6)$$

and for a single element

$$E\left[\frac{2}{n} \left\{ \frac{1}{2} \hat{j} \right\}^2\right] = \frac{1}{4} (\sigma^2(i-) + \sigma^2(i+)) \quad (7)$$

It follows that

$$E[S(i-)] = \left(\frac{1}{2} n - l - \frac{3}{4} m\right) \sigma^2(i-) + \frac{1}{4} m \sigma^2(i+) \quad (8)$$

$$E[S(i+)] = \left(\frac{1}{2} n - l - \frac{3}{4} m\right) \sigma^2(i+) + \frac{1}{4} m \sigma^2(i-) \quad (9)$$

If we now define

$$s^2(i-) = S(i-) / \left(\frac{1}{2} n - l - \frac{1}{2} m\right) \quad (10)$$

then

$$E[s^2(i-)] = \sigma^2(i-) + \frac{m}{2n - 4l - 2m} (\sigma^2(i+) - \sigma^2(i-)) \quad (11)$$

and similarly for $s^2(i+)$ with the roles of $\sigma^2(i-)$ and $\sigma^2(i+)$ reversed.

3.4. Some Illustrations with the 8 x 8 Array

The general situation may be better understood by considering a few special cases again using for illustration the 8 x 8 factorial array. Setting $i = 4 = C$, suppose we wish to obtain the dispersion effect $s^2(4-)/s^2(4+)$ which contrasts the variances of the first four and last four observations.

Elimination of Grand Mean: Elimination of the mean (which would usually be unknown) results in the removal of $\hat{0}$ in equations (4). For the 8 x 8 array, $n = 8$, $l = 0$, $m = 1$

$$s^2(4-) = \left\{ \frac{1}{16} [(\hat{4})^2 + (\hat{1} - \hat{5})^2 + (\hat{2} - \hat{6})^2 + (\hat{3} - \hat{7})^2] \right\} / (7/2)$$

and using (11)

$$E[s^2(4-)] = \sigma^2(4-) + \frac{1}{14} [\sigma^2(4+) - \sigma^2(4-)]$$

It will be seen that the slight bias in the variance estimate arises because the isolated effect $\hat{4}$ is a function of all eight observations.

Elimination of the Mean and of Effect $\hat{4}$: If the location effect associated with factor 4 is eliminated as well as the overall mean then a complete pair is removed in (5) and in this example

$$s^2(4-) = \frac{1}{16} \{(\hat{1} - \hat{5})^2 + (\hat{2} - \hat{6})^2 + (\hat{3} - \hat{7})^2\} / 3$$

$$E[s^2(4-)] = \sigma^2(4-)$$

No bias now occurs because elimination of $\hat{0}$ and $\hat{4}$ is equivalent to eliminating means separately from the first four and the last four observations, and $s^2(4-)$ becomes a function of only the first four observations. Similar effects are found with all bracketed pairs. Thus if we eliminate factor 2 and the interaction $2 \cdot 4 = 6$ the bias term does not appear because allowance is being made for different effects of factor 2 at the two levels of factor 4.

In the circumstances of effect sparsity here considered, the bias term in (11) involving $\sigma^2(i+) - \sigma^2(i-)$ would usually be rather small. For example, suppose, with a

design having $n = 16$ runs, that $l = 2$ and $m = 1$, then the bias term will be $\{\sigma^2(i+) - \sigma^2(i-)\}/22$. It seems reasonable to conclude that for purposes of model identification the elimination of location effects by simply taking residuals is unlikely to mislead.

However, if desired, appropriate linear combinations of equations (8) and (9) will yield unbiased estimates $\hat{s}^2(i-)$ and $\hat{s}^2(i+)$ as follows:

$$\hat{s}^2(i-) = s^2(i-) + \frac{m}{2n-4l-4m} (s^2(i-) - s^2(i+))$$

$$\hat{s}^2(i+) = s^2(i+) + \frac{m}{2n-4l-4m} (s^2(i+) - s^2(i-))$$

3.5. Dispersion Interactions

Since more than one dispersion effect might be present we need to consider the possibility of interaction. If the effect of changing from the minus level to the plus level of a factor i is to multiply the variance by ϕ_i irrespective of whether the plus or minus level of factor j is employed we shall say that there is no dispersion interaction between i and j . In such a case the variances for the various factor combinations are as follows

j	+	$\sigma^2(i-, j+) = \phi_j \sigma^2$	$\sigma^2(i+, j+) = \phi_i \phi_j \sigma^2$
	-	$\sigma^2(i-, j-) = \sigma^2$	$\sigma^2(i+, j-) = \phi_i \sigma^2$
		-	+
		-	i
			+

Equivalently for the logged variances the dispersion effects will be additive and in this metric dispersion interactions of all orders may be defined in the usual way. It shall be noted that when there is no dispersion interaction the ratio of the average variance at the plus and minus levels for factor i is

$$\frac{\sigma^2(i+, j-) + \sigma^2(i+, j+)}{\sigma^2(i-, j-) + \sigma^2(i-, j+)} = \frac{\phi_i (1 + \phi_j) \sigma^2}{(1 + \phi_j) \sigma^2} = \phi_i$$

and similarly for factor j and ϕ_j . Thus even when there is more than one dispersion effect the simple analysis described above could still be of value as a preliminary analytical device for indicating which factors needed further study. In particular if two factors

i and j appeared to exhibit dispersion effects, then further analysis would be appropriate to consider the general evidence for activity of these effects taking account also of possible interaction. This could be done by considering general differences among the sums of squares associated with the four cells $S(i-,j-)$, $S(i-,j+)$, $S(i+,j-)$, $S(i+,j+)$ of the two-way table for the two factors. As before these sums of squares would be calculated from residuals after eliminating location effects. The consequences of doing this is explored in the Appendix which gives a matrix generalization of earlier results.

A convenient function for comparing a set of variances s_1^2, \dots, s_k^2 having v_1, \dots, v_k degrees of freedom respectively is Bartlett's criterion,

$$M = N \ln \left(N^{-1} \sum_{t=1}^k v_t s_t^2 \right) - \sum_{t=1}^k v_t \ln s_t^2, \quad \text{where } N = \sum_{t=1}^k v_t.$$

When, as would frequently be the case, the screening design is of only moderate size one could not expect to study simultaneously a large number of factors in this way. For example, for $n = 16$, the individual cells from which $S(i-,j-)$, $S(i-,j+)$, etc. would be calculated will each contain only four observations. However when, in circumstances of effect sparsity, only a very few such effects are likely to be of appreciable magnitude, the above analysis could be of value.

We again illustrate with the welding data. Figure 3(a) shows the 35 distinct values of M computed for the data. There are $\binom{15}{2} = 105$ ways of choosing two columns from the 15 columns of the design but these are aliased in sets of three (any column is the product of two other columns). Thus the largest value is associated with columns $15 = C$, $2 = H$, and $13 = J$. This effect could equally well be attributed to factors C and H with interaction $-CH = J$ or to C and J with interaction $-CJ = H$ or to H and J with interaction $-HJ = C$. It is noteworthy however that the seven largest values of M which stand out from the rest all include factor C in their triplets. Also if the dispersion effect of C is eliminated by rescaling the residuals the plot (Fig. 3(b)) no longer shows outstanding points.

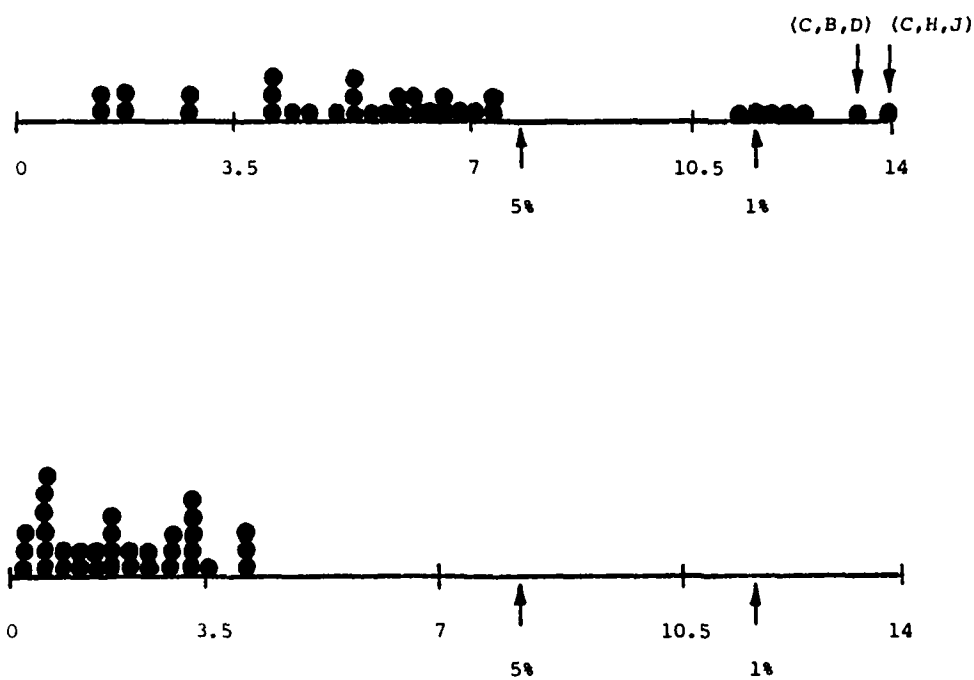


Figure 3. Values of M for distinct column triplets (a) before (b) after elimination of the possible dispersion effect due to factor C. As a rough guide the normal theory 5% and 1% significance levels of M are shown although as before they are not formally justifiable.

4. MAXIMUM LIKELIHOOD ESTIMATES OF LOCATION AND DISPERSION EFFECTS

Once a model has been identified a more precise fitting is possible using maximum likelihood. Hartley and Jayatilake (1973) have shown that the following method will give convergence to a stationary point of the likelihood. Conditional on the dispersion effects, location effects may be obtained by weighted least squares; the dispersion effects may now be recomputed from the residuals and the iteration continued until convergence is achieved. It is often convenient to assume initially that there are no dispersion effects.

For illustration the following table shows maximum likelihood estimates for the welding data assuming location effects for B and C and a dispersion effect for C. The earlier approximate estimates are indicated for comparison.

	μ	\hat{B}	$-\hat{C}$	$\hat{\sigma}^2_{(C-)}$	$\hat{\sigma}^2_{(C+)}$	$\frac{\hat{\sigma}^2_{(C-)}}{\hat{\sigma}^2_{(C+)}}$
Maximum likelihood estimates	42.96	2.04	3.10	.469	.021	22.3
Earlier approximate estimates	43.00	2.15	3.10	.564	.031	18.2

Table 2. Estimates of location and dispersion affects: welding data.

Appendix

The results of section 3 can be generalized to two variables using matrix algebra. Again, \tilde{X} is a matrix of ± 1 's with orthogonal columns $\tilde{x}_0, \dots, \tilde{x}_{n-1}$, \tilde{y} is the vector of observations, and $\hat{j} = \tilde{x}_j \tilde{y}$. Define $I(*)$ to be a $n \times n$ diagonal matrix with 1's in those rows for which the condition $*$ is true, 0's elsewhere. Then, for example, $I(i-)$ is diagonal with 1's in rows where $\tilde{x}_i = -1$; $I(i-, j-)$ is diagonal with 1's in rows where $\tilde{x}_i = \tilde{x}_j = -1$; I is the identity matrix. The following four identities,

$$S(i\pm) = (I(i\pm)\tilde{y})'(I(i\pm)\tilde{y})$$

$$\tilde{I} = \frac{1}{n} \tilde{X}\tilde{X}'$$

$$X_1'X = (I - 2I(i-))X$$

$$I = I(i-) + I(i+)$$

imply, after some algebra, the previously shown identity,

$$S(i-) = \frac{1}{4n} \sum_{j=0}^{n-1} (\hat{j} - i \cdot \hat{j})^2.$$

Extending to two variables, the additional identity

$$S(i\pm, j\pm) = (I(i\pm, j\pm)X)'(I(i\pm, j\pm)X)$$

implies

$$S(i-, j-) = \frac{1}{16n} \sum_{k=0}^{n-1} (\hat{k} - i \cdot \hat{k} - j \cdot \hat{k} + i \cdot j \cdot \hat{k})^2$$

$$S(i-, j+) = \frac{1}{16n} \sum_{k=0}^{n-1} (\hat{k} - i \cdot \hat{k} + j \cdot \hat{k} - i \cdot j \cdot \hat{k})^2$$

$$S(i+, j-) = \frac{1}{16n} \sum_{k=0}^{n-1} (\hat{k} + i \cdot \hat{k} - j \cdot \hat{k} - i \cdot j \cdot \hat{k})^2$$

$$S(i+, j+) = \frac{1}{16n} \sum_{k=0}^{n-1} (\hat{k} + i \cdot \hat{k} + j \cdot \hat{k} + i \cdot j \cdot \hat{k})^2.$$

Now to compute expectations of these quantities, suppose that Z is the $n \times p$ matrix of columns of X which correspond to location effects included in the model, i.e., eliminated to obtain residuals. Then, assuming $E[Y] = Z\tau$, and using the identity

$$E[Y'AY] = \text{trace} (AE[YY'])$$

for A symmetric,

$$E[S(i-, j-)] = \frac{n-2p}{4} \sigma^2(i-, j-) + \frac{1}{2} \sum \text{trace} [ZZ'I(i-, j-)ZZ'I(i\pm, j\pm)] \sigma^2(i\pm, j\pm)$$

where summation is over the four possible combinations of $i\pm, j\pm$. To compute the trace in the above expression, we divide the columns of Z into four groups:

Group 4: Those columns z_k such that $x_i \cdot z_k$, $x_j \cdot z_k$ and $x_i \cdot x_j \cdot z_k$ are also in Z .

Group 3: Those columns z_k such that exactly two of $x_i \cdot z_k$, $x_j \cdot z_k$, $x_i \cdot x_j \cdot z_k$ are also in Z .

Group 2: Those columns z_k such that only one of $x_i \cdot z_k$, $x_j \cdot z_k$, $x_i \cdot x_j \cdot z_k$ is also in Z .

Group 1: Those columns not in previous three groups.

Let m_k = number of columns in group k ; note that m_k is a multiple of k . Further subdivide group 2 into three subsets

Group 2.1: those pairs z_g, z_k with $z_g = x_i \cdot z_k$

Group 2.2: those pairs z_g, z_k with $z_g = x_j \cdot z_k$

Group 2.12: those pairs z_g, z_k with $z_g = x_i \cdot x_j \cdot z_k$.

Let $m_{2,k}$ be the number of columns in group 2.k; $m_2 = m_{2,1} + m_{2,2} + m_{2,12}$.

Then after some algebra,

$$\begin{aligned} E[S(i-, j-)] &= \sigma^2(i-, j-) \left[\frac{4n - 7p + 3m_4 + 2m_3 + m_2}{16} \right] \\ &+ \sigma^2(i-, j+) \left[\frac{p - m_4 - \frac{2}{3}m_3 - m_2 + 2m_{2,1}}{16} \right] \\ &+ \sigma^2(i+, j-) \left[\frac{p - m_4 - \frac{2}{3}m_3 - m_2 + 2m_{2,2}}{16} \right] \\ &+ \sigma^2(i+, j+) \left[\frac{p - m_4 - \frac{2}{3}m_3 - m_2 + 2m_{2,12}}{16} \right] \end{aligned}$$

Note that $S(i-, j-)$ will be unbiased (up to a scale factor) if all columns of Z are in group 4 ($p = m_4$, $m_3 = m_2 = m_1 = 0$) i.e. for each variable x_k eliminated, variables

$x_{i \cdot k}$, $x_{j \cdot k}$, $x_{i \cdot j \cdot k}$ are also eliminated. Similar expressions for expectations of $S(i-, j+)$, $S(i+, j-)$ and $S(i+, j+)$ can be worked out quite easily from the above formula

by switching signs on i, j . In particular, the expression for $E[S(i-)]$ derived in section 3.3 follows immediately with

$$\sigma^2(i-) = \frac{1}{2} (\sigma^2(i-, j-) + \sigma^2(i-, j+))$$

$$\sigma^2(i+) = \frac{1}{2} (\sigma^2(i+, j-) + \sigma^2(i+, j+)) .$$

Thus the calculation of estimated dispersion effects defined as the change in the average variance is not affected by the existence of more than one real dispersion effect.

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